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ADP012127

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# CHEMICAL-KINETIC CHARACTERIZATION OF AUTOIGNITION AND COMBUSTION OF DIESEL AND JP-8

(Grant/Contract Number DAAD19-99-1-0259)

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## SUMMARY/OVERVIEW:

The principal objective of the research is to obtain a fundamental understanding of the mechanisms of autoignition and combustion of diesel and JP-8. Chemical-kinetic mechanisms describing autoignition and combustion of these fuels are not available. This research will address this deficiency by first developing simulated diesel and simulated JP-8 each preferably made up of three hydrocarbon compounds. Chemical-kinetic mechanisms will be developed for these hydrocarbon fuels. Experimental and numerical studies are in progress.

## TECHNICAL DISCUSSION:

Numerical and analytical studies were carried out to elucidate the ignition characteristics of premixed mixtures of *n*-heptane and air in homogeneous, nonflowing systems. In particular two-stage ignition characteristics of the reactive mixture was investigated. The results are described in Ref. 1. Chemical-kinetic mechanisms of combustion of propene ( $C_3H_6$ ), and ethene ( $C_2H_4$ ) are considered to be subsets of chemical-kinetic mechanism of combustion of *n*-heptane. To test the accuracy of these subsets, experimental and numerical studies were carried out to elucidate the fundamental mechanisms of extinction and autoignition of propane ( $C_3H_8$ ), propene, ethane ( $C_2H_6$ ), and ethene in nonpremixed systems. The results are reported in Ref. 2. Alkylated benzenes are an important class of hydrocarbons because they comprise a significant portion of diesel. Knowledge of the oxidation chemistry of alkylated benzenes is needed in developing predictive models that can treat autoignition, and premixed and nonpremixed burning of transportation fuels in internal combustion engines. Toluene ( $C_6H_5CH_3$ ) has the simplest molecular structure of the alkylated benzenes and is a reasonable starting point for the development of detailed chemical-kinetic mechanisms for alkylated benzenes. An experimental and numerical study was performed to elucidate the chemical-kinetic mechanism of combustion of toluene. The results are described in Ref. 3.

### *Temperature Cross-Over and Non-Thermal Runway at the Two-Stage Ignition of n-Heptane*

This research was carried out in collaboration with Professor N. Peters and Mr. G. Paczko at RWTH Aachen Germany. Numerous studies have addressed ignition of *n*-heptane in homogeneous, nonflow systems. A particular striking feature is two-stage ignition which is also related to cool flame phenomena and the negative temperature coefficient

(NTC) of the ignition delay time. The procedure used in this study is to first develop a skeletal mechanism made up of minimum number of reaction steps that is able to reproduce ignition delay times in the low and high temperature regime. The skeletal mechanism is obtained from a detailed chemical-kinetic mechanism. Reduced chemical-kinetic mechanisms are obtained from the skeletal mechanism. The reduced chemical-kinetic mechanisms are used to predict ignition delay times.

Two reduced mechanisms are derived for describing the low temperature regime as well as the intermediate temperature regime and the high temperature regime. In these formulations the OH radical is consumed by fast reactions with the fuel until the fuel is depleted. The steady state relations for OH shows the concentration of OH to become very large when the fuel is depleted. Therefore depletion of the fuel is used as a suitable criterion for ignition. In the intermediate temperature regime the first stage ignition is related to a change from chain-branching to chain-breaking as the temperature crosses a certain threshold. The chain branching reactions result in a build-up of ketohydroperoxides which dissociate to produce OH radicals. This is associated with a slight temperature rise which leads to a crossing of the threshold temperature with the consequence that the production of OH radicals by ketohydroperoxides suddenly ceases. The subsequent second stage is driven by the much slower production of OH radicals owing to the dissociation of hydrogen peroxide. In all three regimes analytical solutions for the ignition delay are obtained. It is found that dissociation of the ketohydroperoxide dominates the low temperature regime and the first stage ignition of the intermediate temperature regime, while dissociation of hydrogen peroxide dominates the second stage of the intermediate temperature regime and the high temperature regime.

*Experimental and Numerical Studies of Extinction and Autoignition of  $C_3H_8$ ,  $C_3H_6$ ,  $C_2H_6$ , and  $C_2H_4$*

This research was carried out in collaboration with Dr. W. J. Pitz at Lawrence Livermore National Laboratory, Livermore California. Experimental and numerical studies are conducted to clarify the physical and chemical mechanisms of extinction and autoignition of ethene, ethane, propene, and propane. The studies are performed in the counterflow configuration. Here the reactive layer stabilized near the stagnation plane of two counterflowing streams is considered. Nonpremixed and premixed systems are considered. In nonpremixed systems one stream, called the fuel stream, is made up of fuel and nitrogen, and the other stream, called the oxidizer stream, is made up of air mixed with nitrogen. In premixed systems one stream, called the premixed reactant stream, is made up of ethene, air and nitrogen, and the other stream, is made up of nitrogen.

Critical conditions of extinction of nonpremixed flames, giving the mass fraction of various reactants in the streams as functions of strain rates, are obtained. In the autoignition experiments on nonpremixed systems, at a fixed value of the strain rate, the temperature of the oxidizer stream was increased until spontaneous ignition took place. Autoignition temperatures are obtained for several values of the strain rate. Experimental results are shown in Fig. 1. Studies on premixed systems are carried out with ethene as the fuel. One series of experiments gives strain rates at extinction for different equivalence ratios

and dilutions of the premixed reactant stream. Here, the nitrogen stream is at ambient temperature. In the second series of experiments, strain rates at extinction are obtained as a function of the nitrogen stream temperature.

Numerical calculations are performed using detailed chemistry at several conditions corresponding to those in the experiments. Critical conditions of extinction and autoignition are calculated. The numerical results are compared with the experiments.

#### *Chemical-Kinetic Characterization of Combustion of Toluene*

This research was carried out in collaboration with Dr. W. J. Pitz and Dr. C. K. Westbrook at Lawrence Livermore National Laboratory, Livermore California, Prof. J. W. Bozzelli at New Jersey Institute of Technology, Newark, and Dr. I. Da Costa, Dr. R. Fournet, Dr. F. Billaud, and Dr. Battin-Leclerc at CNRS-ENSIC, BP. 451, 1, rue Grandville, 51001 Nancy, France. Here a study is performed to elucidate the chemical kinetic mechanism of combustion of toluene. A detailed chemical-kinetic mechanism for toluene was improved by adding more accurate description of the phenyl + O<sub>2</sub> reaction channels. Results obtained using the chemical-kinetic mechanism are compared with experimental data obtained from premixed and nonpremixed systems. Under premixed conditions, predicted ignition delay times are compared with new experimental data obtained in shock tube. Profiles of a number of chemical species were measured previously in the Princeton atmospheric-pressure flow reactor. These measured profiles are compared with numerical calculations using the chemical kinetic mechanism developed here. Ignition delay times are calculated and compared with previous data obtained in rapid compression machines and shock tubes. Critical conditions of extinction and ignition were measured in strained laminar flows under nonpremixed conditions. Numerical calculations were performed using the chemical kinetic mechanism at conditions corresponding to those in the experiments. Critical conditions of extinction and ignition were obtained and compared with the experimental data. Figure 2 compares experimental data on autoignition with results of numerical calculations. For both premixed and nonpremixed systems, sensitivity analysis was used to identify the reaction rate constants that control the overall rate of oxidation in each of the systems considered.

#### *References*

- [1] N. Peters, G. Paczko, R. Seiser, and K. Seshadri, "Temperature Cross-Over and Non-Thermal Runway at Two-Stage Ignition of *n*-Heptane," submitted for publication in *Combustion and Flame*, March 2001.
- [2] R. Seiser, K. Seshadri, and W. J. Pitz, "Experimental and Numerical Studies of Extinction and Autoignition of C<sub>3</sub>H<sub>8</sub>, C<sub>3</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>6</sub>, and C<sub>2</sub>H<sub>4</sub>," Paper # 149, 2nd Joint Meeting of the U. S. Sections of the Combustion Institute, Oakland, CA, March 25-28, 2001.
- [3] W. J. Pitz, R. Seiser, J. W. Bozzelli, I. Da Costa, R. Fournet, F. Billaud, F. Battin-Leclerc, K. Seshadri, and C. K. Westbrook, "Chemical Kinetic Characterization of Combustion of Toluene," Paper # 252, 2nd Joint Meeting of the U. S. Sections of the Combustion Institute, Oakland, CA, March 25-28, 2001.

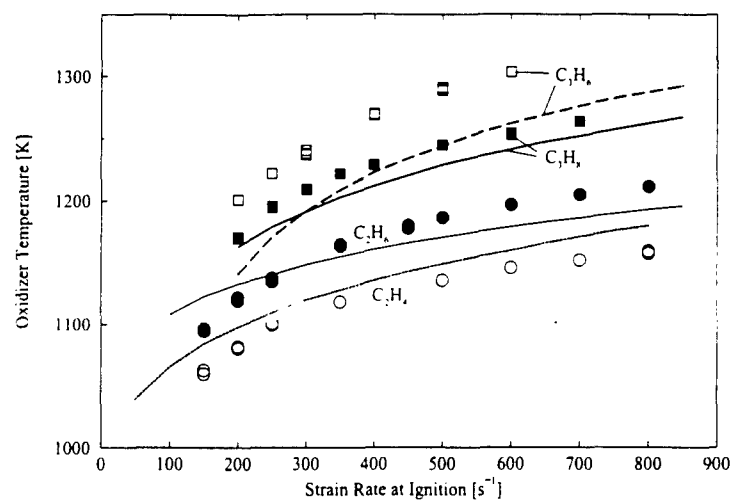


Figure 1: The oxidizer temperature as a function of the strain-rate at autoignition. The points represent measurements and the lines are results of numerical calculations.

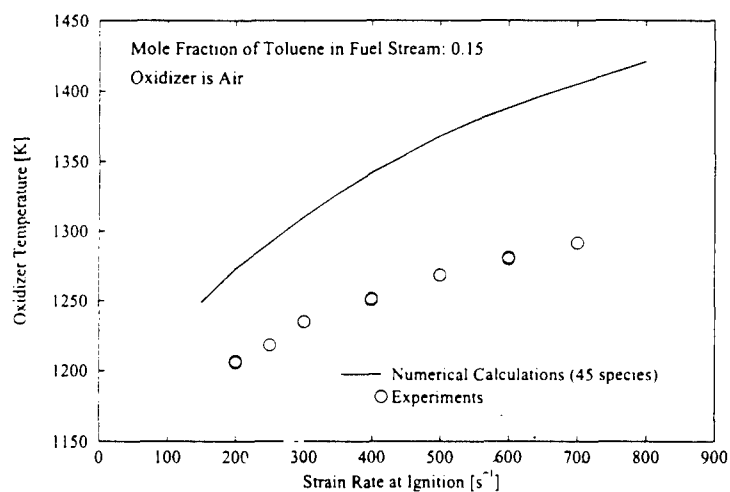


Figure 2: The oxidizer temperature as a function of the strain-rate at autoignition. The points represent measurements and the lines are results of numerical calculations.